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MONTE CARLO SIMULATION OF A KINETIC ISING MODEL OF THE GLASS TRANSITION

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Results of Monte Carlo experiments for the two-spin facilitated kinetic Ising model on a cubic lattice are presented and compared with a theoretical prediction.

IN A RECENT LETTER Fredrickson and Andersen [1] introduced a special kinetic Ising model as a model for structural relaxation in dense liquids and glasses. The Hamiltonian is the usual Ising one with ferromagnetic coupling J between nearest neighbor spins in a magnetic field H which tends to align the spins downwards. As in the Glauber model [2] the dynamics is described by a master equation with transition probabilities satisfying the detailed balance principle. In a special version, the two-spin facilitated model, the down-flip rate of a particular spin σ_j is chosen as

$$w_{j,\text{down}}(\sigma_j) = \alpha m_j(m_j - 1)/2,$$

where m_j is the number of nearest neighbor up-spins of spin σ_j , α sets the time scale and the up-flip rate $w_{j,\text{up}}(\sigma_j)$ is chosen to satisfy the detailed balance condition. Thus the spin flip rate is zero unless σ_j has at least two neighboring up-spins which can facilitate the flipping of σ_j . Fredrickson and Andersen [4] presented arguments, but could not prove, that the Markov chain corresponding to the master equation dynamics is irreducible [3]. If the Markov process is irreducible this model has the same equilibrium properties as the Ising model so that any phase transition in a nonzero magnetic field must be of dynamical origin [1].

Fredrickson and Anderson [1, 4] developed a diagrammatic perturbation theory for this model and by resuming diagrams of leading order in the small concentration c of up-spins, they derived a self-consistent equation for the equilibrium single-spin autocorrelation function $C(t) = [\langle \sigma_i(t)\sigma_i(0) \rangle - \langle \sigma_i \rangle^2] / [1 - \langle \sigma_i \rangle^2]$. In particular they predict that by lowering the concentration c of up-spins the relaxation time τ increases and diverges

at a critical value c^* below which spin fluctuations are frozen as is manifested in $C(t)$ decaying to a nonzero value f ($f^* < f < 1$ for $c^* > c > 0$) in the infinite time limit.

In order to test these theoretical predictions we have performed Monte Carlo experiments [5] for the two-spin facilitated kinetic Ising model with $N = 16^3$ spins on a cubic lattice. To test the size dependence runs were made also for $N = 32^3$, but no significant changes were observed. We chose $J = 0$ since for non-interacting spins equilibrium configurations at a given temperature T and magnetic field H with a concentration of up-spins $c = [1 + \exp(2H/k_B T)]^{-1}$ can be established efficiently. This means that the initial configuration of up- and down spins is random with given concentration c . Furthermore some approximations of the theory [4] become exact in this limit.

The Monte Carlo runs were performed up to 10^4

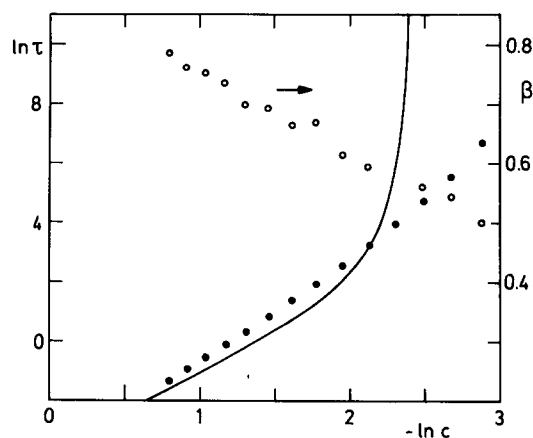


Fig. 1. Relaxation time τ and exponent β versus fraction of up-spins c determined by Monte Carlo simulation compared with theory [1, 4] (full line).

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Monte Carlo steps (MCS). We find that $C(t)$ can reasonably well be approximated by a Kohlrausch law [6] $\Phi(t) = \exp(-(t/\tau)^\beta)$ in the time regime $6 < t < 60$ (α is chosen so that 100 MCS correspond to 6 time units of [1, 4]) with $\beta = \beta(c)$ as shown in Fig. 1. The fitted τ is expected to show the same qualitative behavior as the one defined by the time integral of $C(t)$. In qualitative agreement with the theory we find that τ increases when the temperature is lowered, as is shown in Fig. 1. However, the relaxation time does not diverge at the predicted value $c^* = 0.0904$, where $f^* = 2/3$. It is interesting to note that an improvement of the theory [4] yields a lower value $c^* = 0.0681$, where $f^* = 0.71$. Our results, however, show no indication of a divergency at this concentration either. In order to locate the experimental value of c^* runs were performed for $c = 0.0474$ and $c = 0.0266$ for times up to $t = 6000$, but even in this time regime $C(t)$ did not settle to a constant nonzero value f .

Summarizing our results we find that the relaxation time increases with decreasing c but we do not find a

diverging τ in the regime predicted by theory [1, 4], a divergency at lower values of c cannot be ruled out, however. If a nonzero value of c^* exists, it is at least three times smaller than predicted by the theory [1, 4].

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REFERENCES

1. G.H. Fredrickson & H.C. Andersen, *Phys. Rev. Lett.* **53**, 1244 (1984).
2. R.J. Glauber, *J. Math. Phys.* (N.Y.) **4**, 294 (1963).
3. J.M. Hammersley & D.C. Handscomb, *Monte Carlo Methods*, Methuen, London, (1964).
4. G.H. Fredrickson & H.C. Andersen, preprints.
5. K. Binder & D. Stauffer, *Applications of the Monte Carlo Method in Statistical Physics*, (Edited by K. Binder) Springer, Berlin, (1984).
6. R. Kohlrausch, *Ann. Phys.* (Leipzig), **12**, 393 (1847).